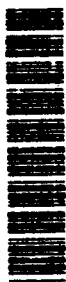


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Low Energy Electron/Atom Elastic Scattering Cross Sections from 0.1-30 keV.

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Abstract

Empirical forms for electron/atom scattering cross sections predict backscattering factors that compare well with those calculated using tabulated Mott data from 0.1 to 30keV. The form of the empirical total cross section is similar to the screened Rutherford cross section. The fit to the tabulated differential Mott cross sections is decomposed into two parts, one part being of the same mathematical form as the screened Rutherford cross section (σ_R), and the second part being an isotropic distribution (σ_I). The ratio of the total cross sections (σ_R/σ_I) between the screened Rutherford part of the differential scattering cross section and the isotropic part of the distribution, is fitted to give the same ratio of forward to backscattered currents as the tabulated Mott differential cross sections. The three equations, one for the total elastic cross section and two equations describing the differential cross section, one for the Rutherford screening parameter and one for the ratio σ_R/σ_I , give backscattering results covering all the major trends with energy and atomic number compared to the backscattering coefficients calculated using tabulated Mott cross sections. However, agreement with experiment is poor for some well

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researched examples such as Au. Monte Carlo calculations using the empirical cross sections show that surface effects may be critical in interpreting experimental results.

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I. Empirical Scattering Cross Sections.

Monte Carlo simulations of electron scattering in a target normally use one of two elastic cross sections, either the screened Rutherford cross section or tabulated partial wave expansions of the Mott cross section. The screened Rutherford cross section gives acceptable results for high energies and low atomic numbers but Mott cross sections are required for low to medium incident energies (0.1-30keV) and high atomic number targets. However, the data set for the tabulated Mott cross sections is large and computations tend to be slow due to the need to interpolate between data points. Because the Mott cross section is itself a complex function of electron energy, atomic number and scattering angle, empirical equations fitted directly to tabulated Mott cross sections are also complex and have not found wide application¹. Recently published empirical equations for the total and differential electron/atom elastic scattering cross sections are based on the observation that multiple scattering of electrons in a solid averages out many of the complex effects in the cross section. These empirical equations are simple and can be easily substituted for the Rutherford cross section in computer code².

The empirical total elastic scattering cross section was derived by fitting to trends in tabulated Mott cross section data and then adjusting parameters to improve calculated backscattering factors in comparison to those calculated using the tabulated Mott data³. The empirical total cross section is a similar form to the screened Rutherford cross section but contains three terms in energy in the denominator; one linear term with an additional square root term and an additional inverse square root term. As the aim of producing empirical fits to electron/atom scattering cross sections is for their use with Monte Carlo calculations it is important to engineer the empirical fit for fast computation. For this reason, the relativistic correction to the cross section was taken inside the fit to reduce the number of terms in energy to be calculated at any step. The empirical total elastic

scattering cross section is valid for atomic numbers up to 92 and for energies from 100eV to 30keV:

$$\sigma_T = \frac{3.0 \times 10^{-18} Z^{1.7}}{(E + 0.005Z^{1.7}E^{0.5} + 0.0007Z^2/E^{0.5})} \text{ cm}^2 \quad (1)$$

The empirical differential cross section is decomposed into two parts, one part being of the same mathematical form as the screened Rutherford cross section (σ_R), and the second part being an isotropic distribution (σ_I). The Rutherford and the isotropic forms were chosen for the differential cross section because they give simple analytical forms for the random generation of scattering angles. The screened Rutherford part of the differential cross section was fitted to the half angles at half heights of the tabulated Mott differential cross section. This fit of the differential screened Rutherford was in turn reduced to a fit of the screening parameter alone over energy and atomic number. In marked contrast to the screened Rutherford cross section, the tabulated Mott cross sections show only a small overall downward trend in half angle with increasing atomic number (Z). This small variation occurs because the low-angle forward scattering is dependent on the size of the atom, not the size of the nucleus. Atom sizes are similar across the periodic table except where different electron shells are filled or not. However, the half angles are sensitive to the atomic model used, and also show large variations with atomic number. The empirical fit ignores all the variations due to shell sizes, and all changes with Z . However, forward scattering is largely dominated by the density of the material and computation shows that transmission through foils is not sensitive to changes in half angle similar to the possible inaccuracies as long as the total cross section or the Rutherford to isotropic cross-section ratios are adjusted to compensate. The average half angles for low atomic numbers are 7° and show a minimum at higher atomic numbers of

around 5° . The average value is 6° which implies a Rutherford screening parameter for all Z of:

$$\alpha = 7.0 \times 10^{-3} / E \quad (2)$$

where E is the electron energy.

The screening parameter, α , is only used to define the distribution of the scattering from the Rutherford part of the differential cross section and has no meaning with respect to the total cross section. The scattering angle for the Rutherford part is defined by:

$$\cos(\theta) = 1 - \frac{2\alpha R}{1 + \alpha - R} \quad (3)$$

Where R is a random number between 0 and 1. The scattering angle for the isotropic distribution is:

$$\cos(\theta) = 1 - 2R \quad (4)$$

The screened Rutherford part of the cross section as fitted to the Mott data is highly peaked in the forward scattering direction and needs to be balanced by the isotropic distribution. The ratio of the total cross sections (σ_R / σ_I) between the screened Rutherford part of the differential scattering cross section and the isotropic part of the distribution, was fitted to give the same ratio of forward to backscattered currents as the tabulated Mott differential cross sections. A Monte Carlo simulation was then run and the ratio was adjusted to give a fit to calculated backscattering factors of Czyzewski et al.³ from 0.1 to

20 keV and experimental data of Drescher, Reimer, and Seidel⁴ for Au and Be up to 30keV. The ratio of Rutherford to isotropic cross sections is:

$$\frac{\sigma_{\text{Rutherford}}}{\sigma_{\text{Isotropic}}} = \frac{300E^{1-Z/2000}}{Z} + \frac{Z^3}{3 \times 10^5 E} \quad (5)$$

Note that there is no connection between the total cross section of equation 1 and the differential cross section defined by equations 2 and 5.

Figure 1 shows a comparison of the calculated backscattering factors using the empirical fit (solid lines) with the data of Czyzewski et al.³ The fit for Al, Cu and Au is good over the entire energy range. The fit for Ag is poor in the knee at low energy, which opposes the trends set by Cu and Au. The fit for C is high but the experimentally supported fit at 10 keV and 30 keV for Be⁴ is very good (these two data points not shown). The knee for Au is too high and the knee for Al is too low compared with the Czyzewski et al.³ data. However, these deviations are similar to differences due to the use of different atomic models and don't justify the addition of extra terms in the cross sections.

The exponential energy term in equation 5 can be simplified to a linear dependence. This simplification changes the backscattering factor for Au at 30 keV from 0.5 to 0.48 but is insignificant at lower atomic number and energy.

While equations 1, 2 and 5 are a good description of the overall trends of the Mott elastic cross section with energy and atomic number they do not follow the periodicity of the Mott cross sections which are directly due to the periodic variation of the size of the atom. There are two major reasons why simple monotonic equations work

well. First, the scattering of the electrons in a solid is a multiple scattering process. Thus many of the complex quantum interference effects seen in the differential cross section are averaged out for scattering thorough large angles. Second, the total elastic backscattering is monotonic with atomic number. We define the total elastic backscattering as the product of the total cross section and the ratio of backscattered to forward scattered currents². For the Mott cross section the backscattered part is monotonic and dependent on Z^2 , as predicted by the Rutherford cross section. The monotonic trends in the backscattering cross sections found from the Mott cross sections are not unexpected as the large-angle scattering involves scattering from the central nuclear potential and is thus not a periodic function at high energy. Thus these two factors serve to smooth out the effects of the complex multidimensional cross sectional surface over Z , E , and θ .

II. Calculation of Surface Effects.

The fitted elastic cross section reported here gives backscatter factors in good agreement with those calculated using tabulated Mott cross sections but the comparison with experiment is more difficult, particularly in the region below 10keV. Review of the literature for backscattering⁵ show there is considerable divergence in experimental results. This is especially noticeable for Au where we might expect that experiment would produce consistant data^{6,7,8}, figure 2.

The low energy region is difficult for both theory and experiment. At low energies the elastic mean free path of electron in high atomic number targets is very short and both experiment and calculation could be expected to be influenced by small effects. Experimentally we would expect the nature of the surface, topography and contamination, to influence the electron scattering. For low energies there are several difficulties with the calculations, particularly at energies below 1keV. Here, the elastic cross section is changing form, the assumptions in the inelastic cross section are losing validity (the Joy-

Lou form is used⁹), and solid state effects are becoming important. The calculations of figure 1 do not compensate for the energy loss of electrons as they are scattered out of the solid on the last event and the elastic scattering mean free path can be longer than the stopping distance. However, the effects of surface conditions can be calculated in a relative sense and these calculations do suggest reasons why the comparison to experimental literature is problematic

The calculation of backscattering from Au shows that the backscattering factor can be very strongly influenced by the state of the surface at low energies. The backscattering factor is influenced by the relationship between inelastic and elastic scattering. If an electron loses energy quickly before elastic scattering can influence its path then it penetrates into the solid and is not backscattered. At low energies where the elastic cross section from Au is increasing only slowly, the rate of energy loss is high. In contrast, from a low atomic number atom such as C, the elastic cross section is still increasing in a Rutherford like manner. This means that at low energy ($< 0.2\text{keV}$) the backscattering from C is higher than from Au, as can be seen from figure 1. It also means that electrons that have lost a substantial amount of energy and are on the point of being backscattered from the Au will be scattered more than incoming electrons at higher energies by a layer of low atomic number contamination at the surface. As the mean free paths at below 1keV are so short, just $1\text{-}2\text{nm}$ of low atomic number contamination are sufficient to have a noticeable effect. Figure 3 shows the results of a Monte Carlo calculation of the backscattering factor from a clean Au surface and a surface having 2nm of surface oils of atomic number 2, atomic weight 4 and density 1. This low atomic number contamination is sufficient to reduce the backscattering factor at 1keV by 4% because the contamination is relatively transparent to higher energy incoming electrons, but is as effective at scattering as an additional Au layer for low energy backscattered electrons.

Topography also has a considerable effect on the backscattering factor at low energies. In figure 5 we show the effects of two different topographies; a surface of close spaced 10nm deep 45° V grooves, and a surface of 10nm deep 10nm stepped lines spaced at 10nm. The V grooves tend to enhance the backscattering at all energies, as would be expected, and this enhancement peaks at an energy where the average excitation depth is similar to the groove depth. At higher energies the effect is reduced. The stepped lines reduce the backscattering at low energies because the side walls block the low energy backscattered electrons, but at higher energies the backscattering is enhanced. The enhancement at 2keV for the grooved lines is very noticeable, up 15% from the ideal surface.

It can be seen that the combination of topography of less than 10nm and the presence of 1-2nm of contamination are sufficient to produce similar deviations to those seen from experiment to experiment and to departures from the Monte Carlo calculations. These calculations do not prove that the scatter in any of the experimental results are actually due to these effects, although the deviations from a ideal surface are quite reasonable for a mechanically polished surface in a vacuum typical of a scanning electron microscope. However, the calculations do imply that any experiment should be on atomically clean surfaces in UHV and the surface topography should be measured to 1nm.

Summary

The empirical elastic scattering cross sections given by equations 1, 2 and 5 predict back scattering factors from solids that show all the main features and trends as calculations using tabulated Mott cross sections. These cross sections are monotonic with increasing atomic number and do not follow the periodicity of the atomic models.

The calculation of backscattering from Au shows that the backscattering factor can be very strongly influenced by the state of the surface at low energies. Even monolayer

amounts of low atomic number contamination can change the backscattering below 5keV because there is a crossover in the effectiveness of scattering from high and low atomic number at low energy. These calculations imply that experimental studies should be on atomically clean surfaces in UHV and the surface topography should be measured to 1nm.

Acknowledgments

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Figure Captions.

1. Comparison of calculated backscattering factors using equations 1, 3 and 5 (solid lines) and the calculations of Czyzewski et al.³ using tabulated Mott cross sections (symbols).
2. Experimental measurements of electron backscattering from Au for low energies.
● Thomas and Pattinson, □ Schou and Sorensen, ◆ Bongeler et al.
3. Comparison of low energy backscattering from (a) a clean surface and (b) a surface contaminated with 2nm of atomic weight 2, atomic number 4 and density 1.
4. Comparison of the effect of topography on backscattering factor at low energies. (a) no topography, (b) close packed 45° V grooves. (c) 10nm deep, 10nm wide stepped lines at 10nm spacing.

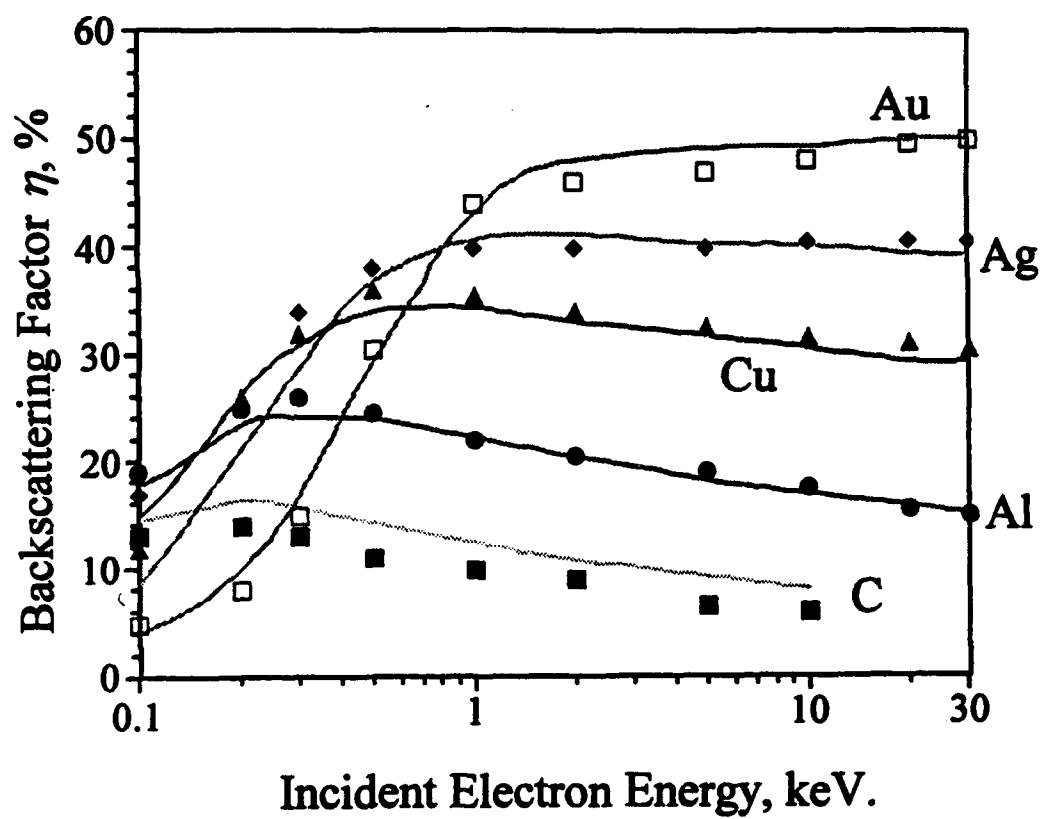


Fig 1

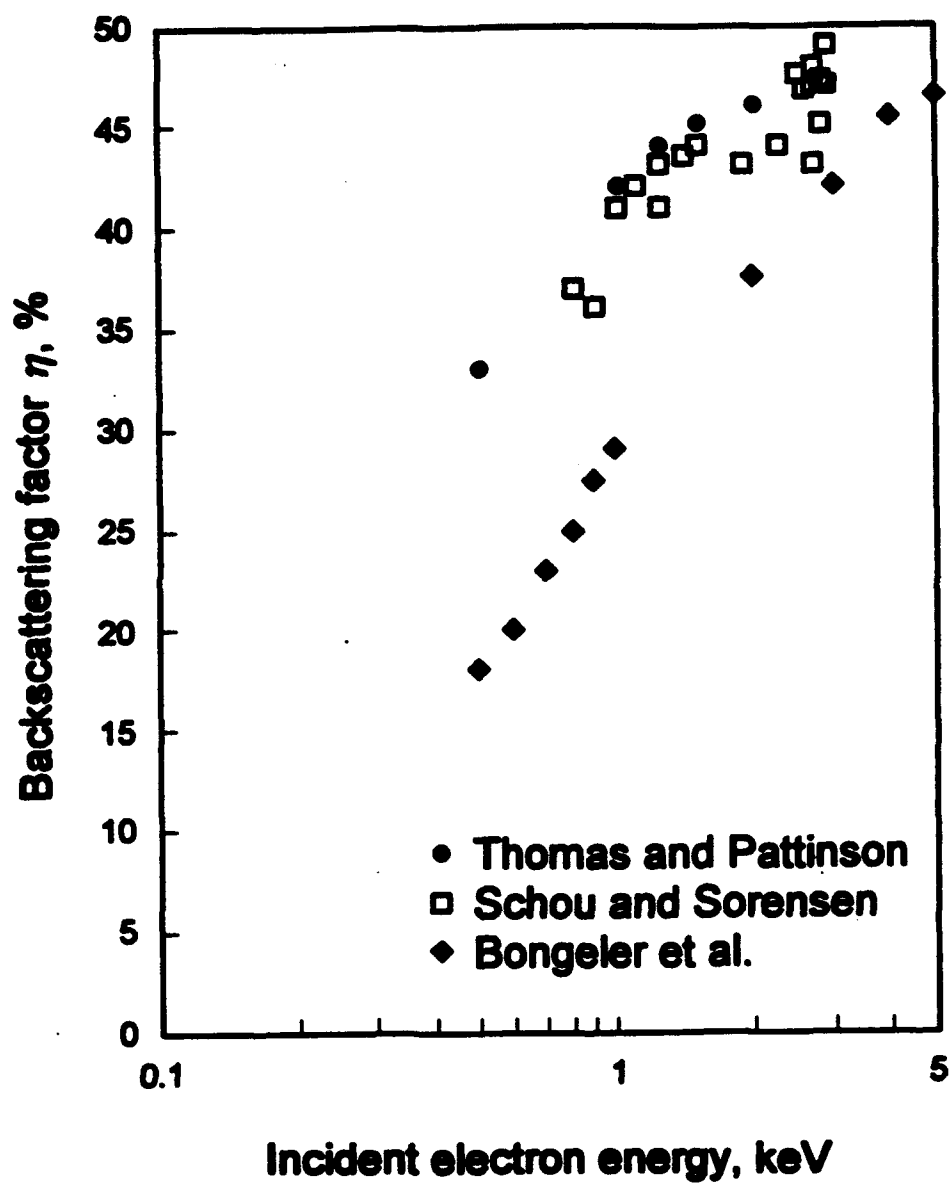


Fig 2

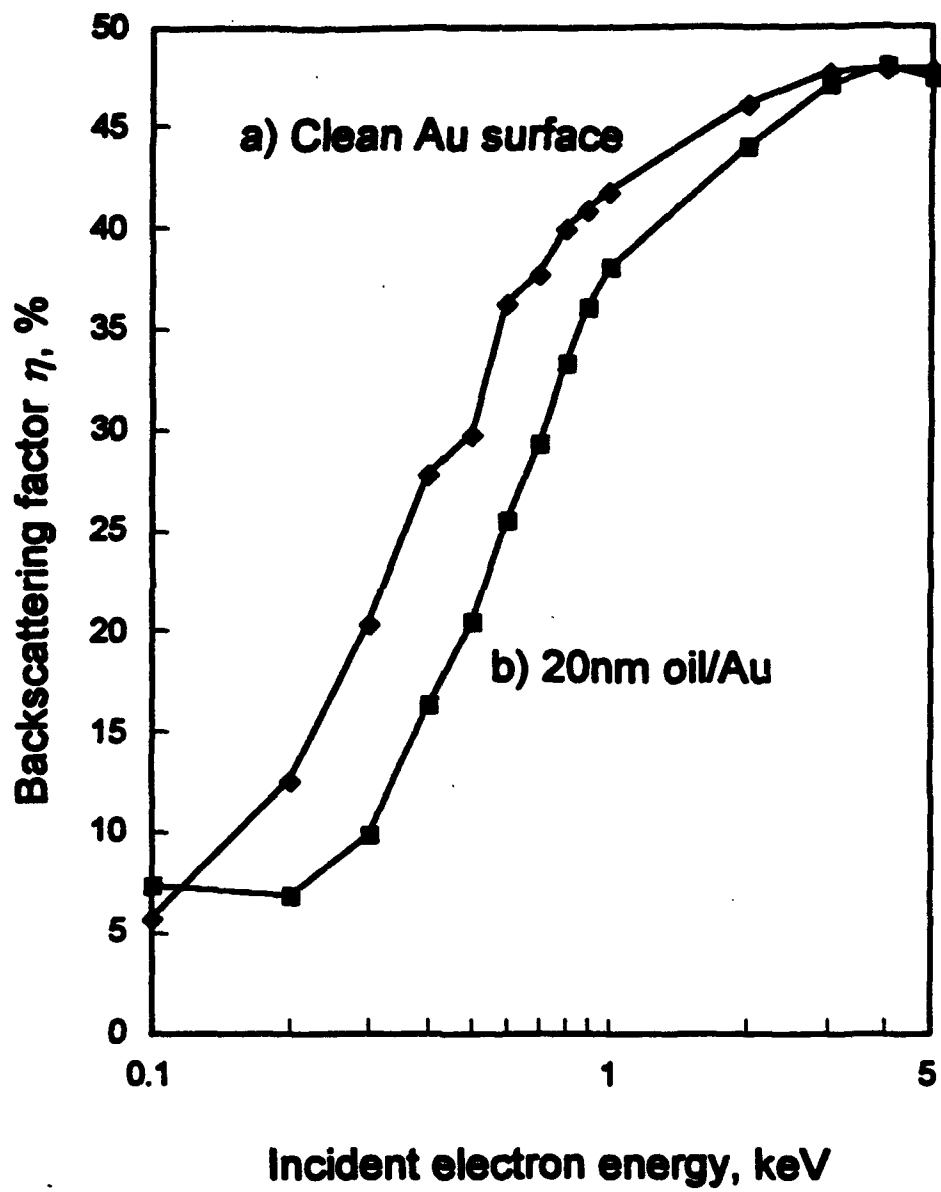


Fig 3

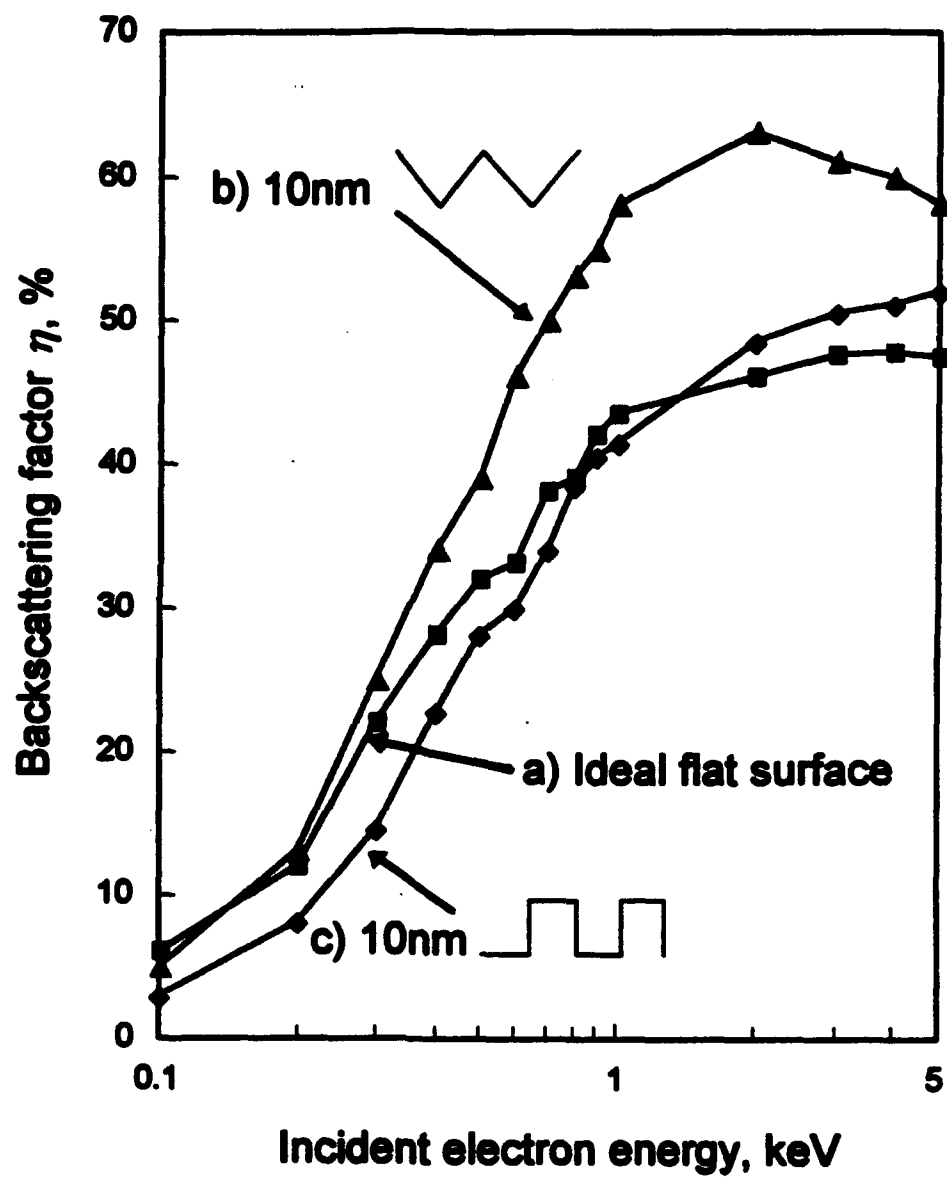


Fig 4